A consistent formalism for the Thomas-Ehrman Level Displacement

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Usage of the Thomas-Ehrman Level Displacement formalism has been examined. Mistakes and inconsistencies are found in several papers, being repeated in subsequent works. Here, we present a complete formalism with a consistent set of definitions. Full algorithms are made available, both as a `FORTRAN` source file and as a user-friendly Visual Basic executable tool, available for download on the World Wide Web.

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I. INTRODUCTION

The Thomas-Ehrman Level Displacement formalism (TELD) [1, 2] is an established technique for calculating the level displacement between mirror pairs. It is found to be particularly useful in situations where a reaction proceeds via a proton resonant state in a proton-rich nucleus. Largely, this usefulness derives from the fact that such states are above the particle decay threshold, usually resulting in proton partial widths too narrow to be measured experimentally. Thus, by appealling to the charge symmetry of the nuclear force, one may make use of relatively abundant spectroscopic data of analogue states in the mirror nucleus to determine the properties of the astrophysically interesting states. Examples in the literature are the ^{21}Ne-^{21}Na [3], ^{20}F-^{20}Na [4], ^{18}O-^{18}Ne [5], ^{22}Ne-^{22}Mg [6] and ^{46}Ti-^{46}Cr [7, 8] mirror nuclear pairs. However, a survey of the literature finds inconsistency in the definition of critical parameters, leading to errors in the calculations. In the present work a complete and consistent TELD formalism is presented and made available for wider use.

II. THE WAVE FUNCTION

Here we reproduce and expand upon the original work of Thomas [2], using, for consistency, exactly the same terminology. The channel radius of two interacting bodies is defined as $a_c = 1.44 \times (A_{1c}^{1/3} + A_{2c}^{1/3})$ fm, with A_{1c} and A_{2c} being the mass numbers of the bodies of the pair; the reduced mass is $M_c = A_{1c}A_{2c}/(A_{1c} + A_{2c})$; the energy of relative motion is ϵ_c, which may be positive or negative. The subscript c is used to describe all of the features of the channel, unless it is necessary to distinguish the positive-energy ($\epsilon_{c+} > 0$) from the negative-energy ($\epsilon_{c-} < 0$) channels in which case the symbols $c+$ and $c-$ are used, respectively.

For external wave functions, a radial factor (Equ. 1 of ref [2]) may be written that satisfies the wave equation

$$\overline{F}_c'' + (2M_c/\hbar^2)(\epsilon_c - \mho_c)\overline{F}_c = 0, \quad (1)$$

where a prime signifies differentiation with respect to r (in the following descriptions, all the derivatives are with respect to r unless stated otherwise). The interaction potential may be written

$$\mho_c = Z_{1c}Z_{2c}e^2 r_c^{-1} + (\hbar^2/2M_c)\ell(\ell+1)r_c^{-2}, \quad (2)$$

where the nuclear potential term disappears in the external region. In the notation of Yost, Wheeler, and Breit [9], the positive-energy solution, which is regular at the origin, is designated by $F(kr)$ and has the asymptotic form for large r,

$$F_{c+} \sim \sin(x - \frac{1}{2}\ell\pi - \eta\ln 2x + \sigma). \quad (3)$$

Likewise, there is a solution which is linearly independent of F and irregular at the origin which is conveniently taken with the asymptotic form for large r,

$$G_{c+} \sim \cos(x - \frac{1}{2}\ell\pi - \eta\ln 2x + \sigma). \quad (4)$$

The quantities entering Equ. 3 and 4 are

$$\begin{aligned} x_{c\pm} &= kr \\ k_{c\pm} &= p/\hbar = (2M_c|\epsilon|/\hbar^2)^{1/2}, \end{aligned}$$

with Sommerfeld parameter

$$\eta_{c\pm} = M_c Z_{1c}Z_{2c}e^2/\hbar^2 k = Z_{1c}Z_{2c}e^2/\hbar v,$$

and

$$\sigma_{c+} = \arg\Gamma(1 + \ell + i\eta).$$

It is worth noting that x is replaced with ρ in some formulations.

The general solution of this equation, $\overline{F}(r)$, is a linear combination of F and G. The Wronskian relation for these two particular solutions, which directly follows from Equ. 1- 4 is

$$F'G - G'F = k_{c+}. \quad (5)$$

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Extensive tables [10] and several computer codes [11, 12, 13] have been developed for evaluating F and G and their derivatives when $\eta > 0$.

For the $c-$ channels, only the solution to Equ. 1, vanishing at large distances from the origin, can occur; it is the Whittaker function [14, 17],

$$W_{-\eta,\ell+\frac{1}{2}}(2x_{c-}) = \frac{e^{-x-\eta \ln 2x}}{\Gamma(1+\ell+\eta)} \int_0^\infty t^{\ell+\eta} e^{-t} \left(1+\frac{t}{2x}\right)^{\ell-\eta} dt. \quad (6)$$

Whittaker function and its derivative may be accurately calculated using the `whittaker_w` [15] computer code. However, it is useful to note that if there is no Coulomb interaction in a $c-$ channel, one has from Equ. 6 for s, p, d, and f orbitals the simpler relations

$$W_{0,\frac{1}{2}}(2x) = e^{-x} \quad (7)$$
$$W_{0,\frac{3}{2}}(2x) = (1+x^{-1})e^{-x} \quad (8)$$
$$W_{0,\frac{5}{2}}(2x) = (1+3x^{-1}+3x^{-2})e^{-x} \quad (9)$$
$$W_{0,\frac{7}{2}}(2x) = (1+6x^{-1}+15x^{-2}+15x^{-3})e^{-x} \quad (10)$$

which can be used for checking the results from a more complicated code.

In discussing conditions at the nuclear surface, one needs to evaluate the real and imaginary parts of the logarithmic derivatives, $g_c = E'/E$, and these are [2],

$$g^{Re}_{c+} = (FF' + GG')(F^2+G^2)^{-1} \quad (11)$$
$$g^{Im}_{c+} = k(F^2+G^2)^{-1} \quad (12)$$
$$g^{Re}_{c-} = W'W^{-1} \quad (13)$$
$$g^{Im}_{c-} = 0 \quad (14)$$

where $g_c = g^{Re} + \mathrm{i}g^{Im}$ and $r_c = a_c$. Although the simple WKB approximation [2, 3] can perform well in calculating the logarithmic derivatives of the Coulomb and Whittaker functions in specified regions, modern computer codes perform essentially exact calculations and are preferred. For example, the difference between the WKB approximation and the exact evaluation of g_{c-}, performed using the code `whittaker_w` [15], in the region $0.1< x <5.0$, $0.1< \eta <10.0$ (roughly corresponding to $Z_{1c}Z_{2c} \leq 20$ and bound nucleon energy $0.1< |E_b| <10.0$ MeV), can be as large as 3% (ℓ=1), 1% (ℓ=2) and 0.6% (ℓ=3), respectively, and becomes smaller as η increases. In the case that ℓ=0, the differences can be as much as 10% when $x <0.1$ and $\eta <0.9$, or $x <0.2$ and $\eta <0.5$, or $x <0.5$ and $\eta <0.3$. In addition, it should be noted that a frequently used subroutine, `COULFG` [12], was unable to reproduce the results (F, G and their derivatives) of the subroutine `RCWFN` near values of $\eta = 1.70x + 5.13$ unless the `ACCUR` variable was set to be less than 10^{-17} (of course the smaller the safer, *e.g.*, 10^{-30} if possible).

III. CALCULATION OF LEVEL DISPLACEMENTS

Under the assumption of charge symmetry of nuclear forces, the nn and pp nuclear interactions are identical. The difference in the excitation energy of levels in mirror nuclei is therefore due to differences in the Coulomb, electromagnetic spin-orbit, and mass energies. As suggested by [2], one can evaluate this by considering $H_p - H_n \equiv V$. Furthermore, in the one-level approximation, irrespective of the boundary conditions, in the internal region the proton and neutron wavefunctions are the same to within a multiplicative constant. Under these assumptions, one obtains (Equ. 30a in ref. [2])

$$E_n - E_p = -\langle V \rangle_\tau + \Delta_{\lambda n} - \Delta_{\lambda p}, \quad (15)$$

where there is a boundary condition that satisfies $\overline{b}_{nc} = \overline{b}_{pc}$ (defined in Equ. 24c of [2]). Here, $\langle V \rangle_\tau$ is the mean value of V in the internal region, and E_n and E_p are the Eigenvalues satisfying $H_{n(p)}\Psi_{n(p)} = E_{n(p)}\Psi_{n(p)}$ of the nucleus with the odd neutron or proton, respectively. The difference of the level displacements of the neutron and proton states (see Equ. 30b of [7]),

$$\Delta_\lambda = \Delta_{\lambda n} - \Delta_{\lambda p} = -\sum_{c\pm} \gamma_c^2 (g^{Re}_{nc} - g^{Re}_{pc}), \quad (16)$$

is referred to as the boundary condition level displacement. The energy difference of corresponding levels of mirror nuclei, following from Equ. 15 and 16, can be written as

$$(E^*_n - E^{g.s.}_n) - (E^*_p - E^{g.s.}_p) = \Delta^*_\lambda - \Delta^{g.s.}_\lambda, \quad (17)$$

where it is assumed that the quantity $\langle V \rangle_\tau$ is the same in the excited state as in the ground state. The scripts $*$ and *g.s.* denote the corresponding quantities are being evaluated with respect to the excited state and the ground state, respectively. Assuming that the level displacements of the two ground states are the same simplifies this relation further,

$$E^*(n) - E^*(p) = \Delta^*_\lambda, \quad (18)$$

where $E^*(n)$ and $E^*(p)$ are the corresponding excitation energies in the mirror nuclei. Therefore, the observed

energy difference between mirror nuclear states is due to different level displacements, $\Delta_{\lambda n}$ and $\Delta_{\lambda p}$, in the two nuclei.

We find that the definitions used by various authors of partial width $\Gamma_{\lambda c}$, reduced width $\gamma^2_{\lambda c}$, dimensionless reduced width $\theta^2_{\lambda c}$ and dimensionless single-particle reduced width θ^2_{sp} [18, 19], of a level λ, are not consistent, as shown in Table I. Following the previous work, the definitions of French [19] are adopted in the present work, though it is possible to achieve consistency using the alternative definitions [2, 20]. One should pay attention that the definition of $\gamma^2_{\lambda c}$ [19] is different from that of [2] by a factor of $3/a_c$. Thus, for the positive-energy channel,

$$-\gamma^2_{c+} g^{Re}_{c+} = -\frac{3\hbar^2}{2M_c a_c^2}\theta^2_{c+} P_c (FF'_x + GG'_x) \qquad (19)$$

with the Coulomb penetrability $P_c = x/(F^2+G^2)$; and for the negative-energy channel,

$$-\gamma^2_{c-} g^{Re}_{c-} = -\frac{3\hbar^2}{2M_c a_c^2}\theta^2_{c-} x\frac{W'_x}{W}. \qquad (20)$$

Where F'_x,G'_x and W'_x represent differentiation with respect to x. Equ. 19 & 20 were defined as Δ_b and Δ_r in previous literature by assuming $\overline{b}_{nc} = \overline{b}_{pc} = 0$ (see Fig. 1).

The reasonable assumption that the reduced widths, γ^2_c, are the same for the mirror levels leads to an assumption of $\theta^2_c = \theta^2_p = \theta^2_n$. Thus, the excitation-energy displacements of mirror nuclei can be expressed as

$$\Delta^*_\lambda = \frac{3\hbar^2}{2M_c a_c^2}\theta^2_c \left\{ [P_c(FF'_x + GG'_x)]_{|E=E_r} - \left(x\frac{W'_x}{W}\right)_{|E=E_b} \right\}, \qquad (21)$$

where E_r [$=E^*(p) - S^p_p$] and E_b [$=|E^*(n) - S^n_n|$] are the energies relative to the respective nucleon thresholds (S^p_p and S^n_n; the superscripts p and n refer to the odd-proton (or proton-rich) and odd-neutron (or neutron-rich) nuclei, respectively; the subscripts p and n denote the corresponding nucleon separation energies). A pictorial representation of the physical meanings of the parameters described here are illustrated in Fig. 1 which shows the case of the 6.424 MeV state in ^{46}Ti and its analogue state in ^{46}Cr [21]. It is clear from the figure that the level displacement may equally well be written as,

$$E^*(n) - E^*(p) = [E^*(n) - S^p_p] - [E^*(p) - S^p_p] = E'_b - E_r, \qquad (22)$$

where the quantity E'_b is different from that of E_b defined above. It appears that confusion over these definitions has, in part, been the source of errors in the past. For example, in several previous works [4, 5, 6, 7] the level displacement has been written as $E^*(n) - E^*(p) = E_b - E_r$ in contrast to the correct expression of $E^*(n) - E^*(p) = E'_b - E_r$ which follows from Marion *et al.* [3]. However, the pressent work validates that the correct expression was used in the calculations [22].

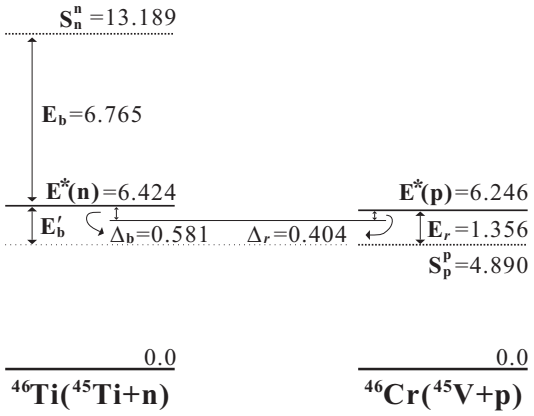

FIG. 1: Definitions and calculation results of relevant quantities in case of the ^{46}Ti-^{46}Cr mirror pair. The calculated values (in units of MeV) are with respect to the analogue states at 6.424 MeV (in ^{46}Ti) and 6.246 MeV (in ^{46}Cr) [21].

The final ingredient which is needed to allow calculation of the level shift is the dimensionless reduced width, θ^2_c. This can be calculated according to the relation θ^2_c=C^{2}Sθ^2_{sp} [18, 19], where the dimensionless single-particle reduced width θ^2_{sp} has already been determined [23, 24], and the factor C^{2}S is calculated via a shell-model code such as `OXBASH` [25].

IV. ONLINE RESOURCES

The algorithms developed here have been made available online [26]. The Visual Basic tool requires the `TELD_VB` and `TELD` executables be in the same directory. Opening the `TELD` application provides a window in which one defines the parameters of the mirror states to be considered (A, Z, S_n, S_p and $E_x(n)$). One also could change values for the channel radius, the orbital angular momentum of the single particle and spectroscopic factor for the state. Activation of the "calc" button then performs the TELD formalism and returns the resulting excitation of the proton-rich analogue state and the proton decay width for this state. This last parameter is calculated using the relation

$$\Gamma_p = \frac{3\hbar^2 P_c \theta^2_p}{M_c a_c^2}. \qquad (23)$$

In addition, a Fortran source code, which allows users to make changes whenever required, is also encloded in the TELD.rar package. Figure 2 shows a screenshot from the `TELD` program with all relevant parameters for the case of the 6.424 MeV state in ^{46}Ti and its analogue state in ^{46}Cr [21].

TABLE I: Various definitions of $\Gamma_{\lambda c}$,$\gamma^2_{\lambda c}$, $\theta^2_{\lambda c}$ and θ^2_{sp} [18, 19] of a level λ in the literature.

	$\Gamma_{\lambda c}$	$\gamma^2_{\lambda c}$	$\theta^2_{\lambda c}$	θ^2_{sp}
Thomas [2]	$2P_c(\gamma^2_{\lambda c}/a_c)$	$\frac{\hbar^2}{2M_c a_c}\theta^2_{\lambda c}$	$a_c \times \frac{u^2(a_c)}{\int_0^{a_c} u^2(r)dr}$	
Lane and Thomas [18, 20]	$2P_c\gamma^2_{\lambda c}$	$\frac{\hbar^2}{M_c a_c^2}\theta^2_{\lambda c}$	$\mathrm{C^2S}\theta^2_{sp}$	$\frac{a_c}{2} \times \frac{u^2(a_c)}{\int_0^{a_c} u^2(r)dr}$
French [19]	$2P_c\gamma^2_{\lambda c}$	$\frac{3\hbar^2}{2M_c a_c^2}\theta^2_{\lambda c}$	$\mathrm{C^2S}\theta^2_{sp}$	$\frac{a_c}{3} \times \frac{u^2(a_c)}{\int_0^{a_c} u^2(r)dr}$

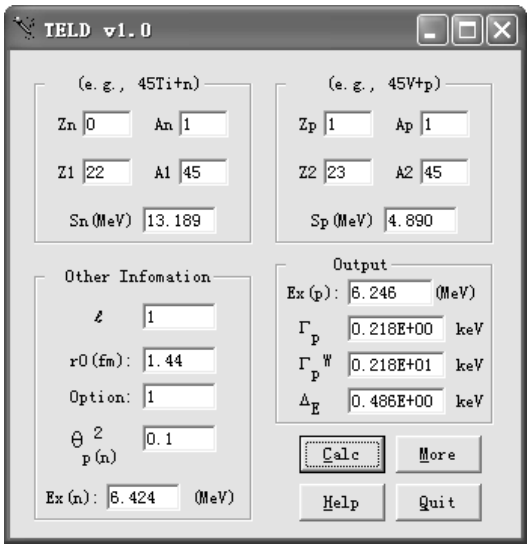

FIG. 2: Screenshot from the TELD program for the case of the 6.424 MeV state in ^{46}Ti and its analogue state in ^{46}Cr [21].

V. SUMMARY

A complete and consistent Thomas-Ehrman Level Displacement formalism has been presented and made available on the World Wide Web. With this, if one has knowledge (or makes a reasonable assumption) of the quantity θ_c^2 and spectroscopic factor S, one may estimate the location of the mirror to a known excited state. Alternatively, experimental measurement of the mirror level displacement provides a route to determining θ_c^2 (or S factor).

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